Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Revisiting the Thermal Decomposition Mechanism of $MAPbI_3$

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The Gibbs free energies were obtained according to the equation:

$$G = E_{ele} + ZPE - TS \quad \text{(S1)}$$

where E_{ele} is the electronic energy of the system in the ground state, T is the temperature (herein we set it to 300 K), S is the entropy of the system obtained from vibrational frequency, and ZPE is the zero-point energy correction.

The reaction energy barriers (G_b) were calculated according to the following equation:

$$G_b = G_{TS} - G_{IS} \quad \text{(S2)}$$

where G_{IS} and G_{TS} are Gibbs free energies of the initial and transition states, respectively.

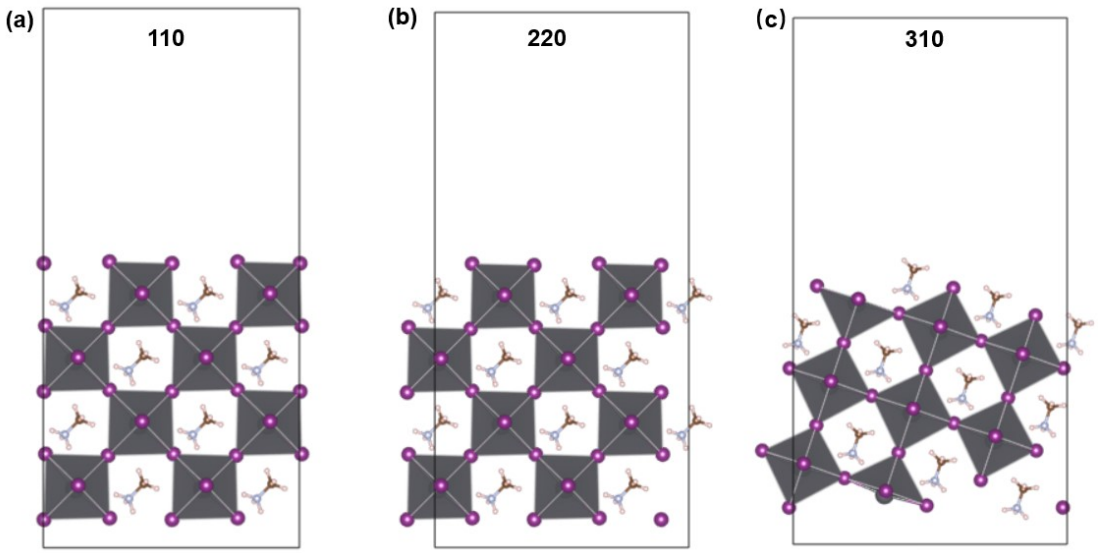

Figure S1 The front views of the optimized $MAPbI_3$ surfaces. (a) (110) surface; (b) (220) surface; (c) (310) surface.

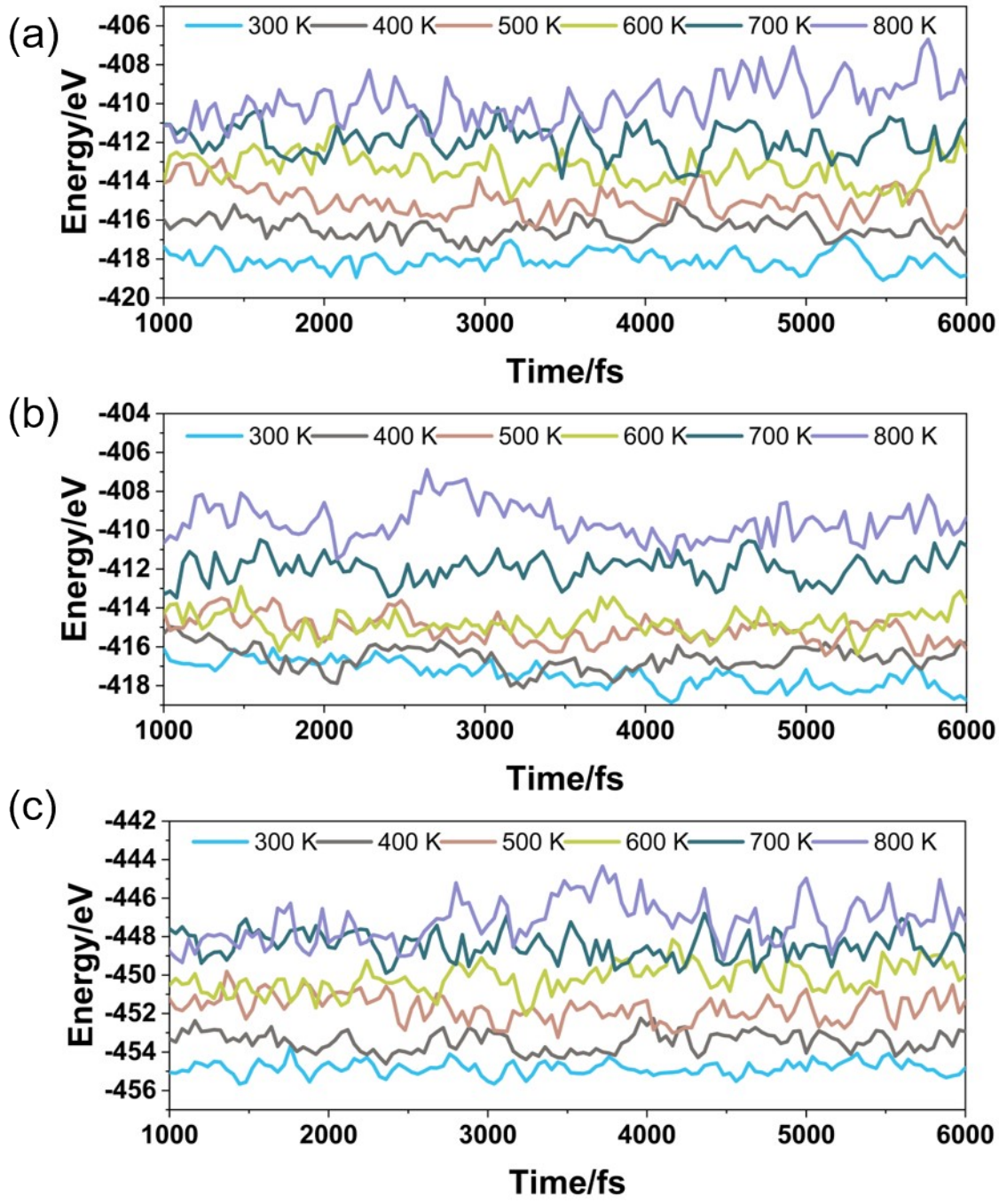

Figure S2 AIMD simulations: energies of $MAPbI_3$ from 300 to 800 K. (a) (110) surface; (b) (220) surface; (c) (310) surface.

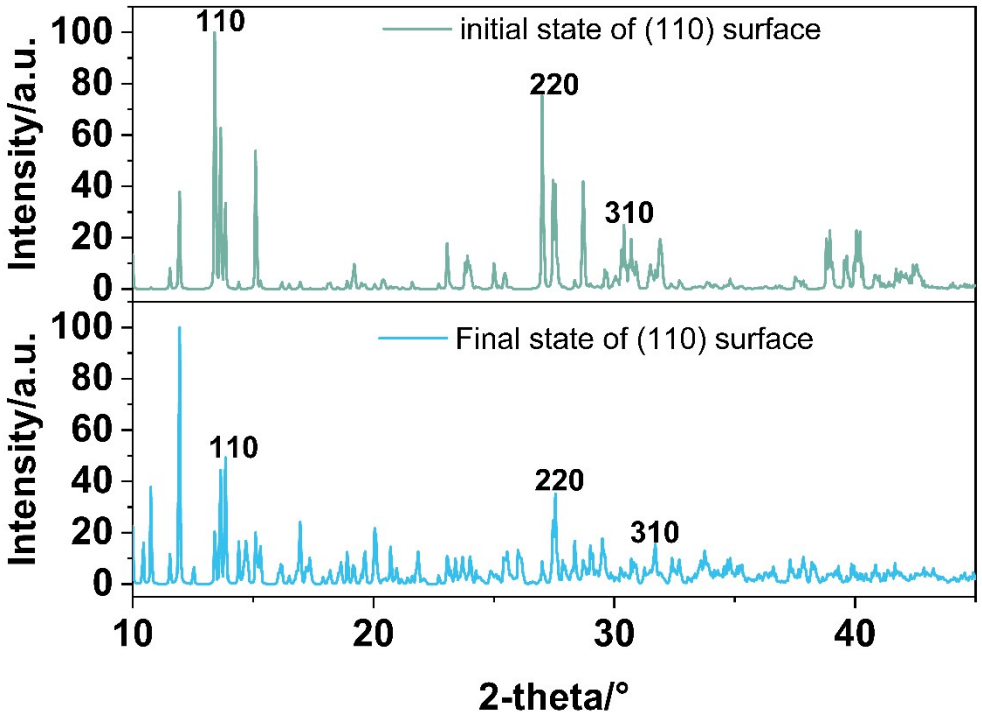

Figure S3 The XRD of (110) surface at 600 K

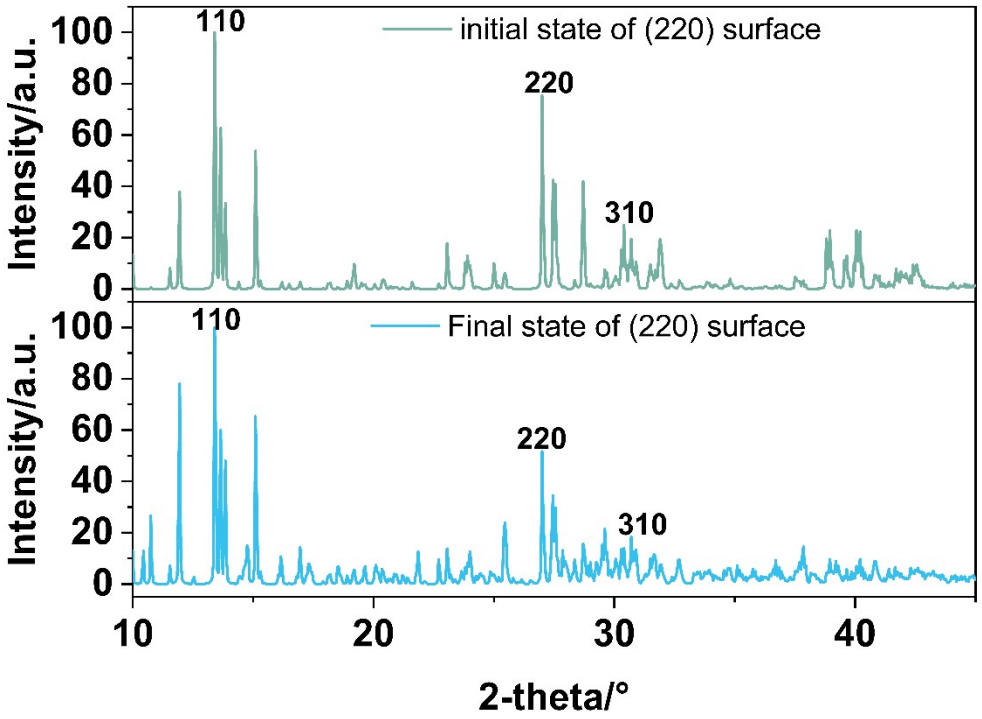

Figure S4 The XRD of (220) surface at 600 K

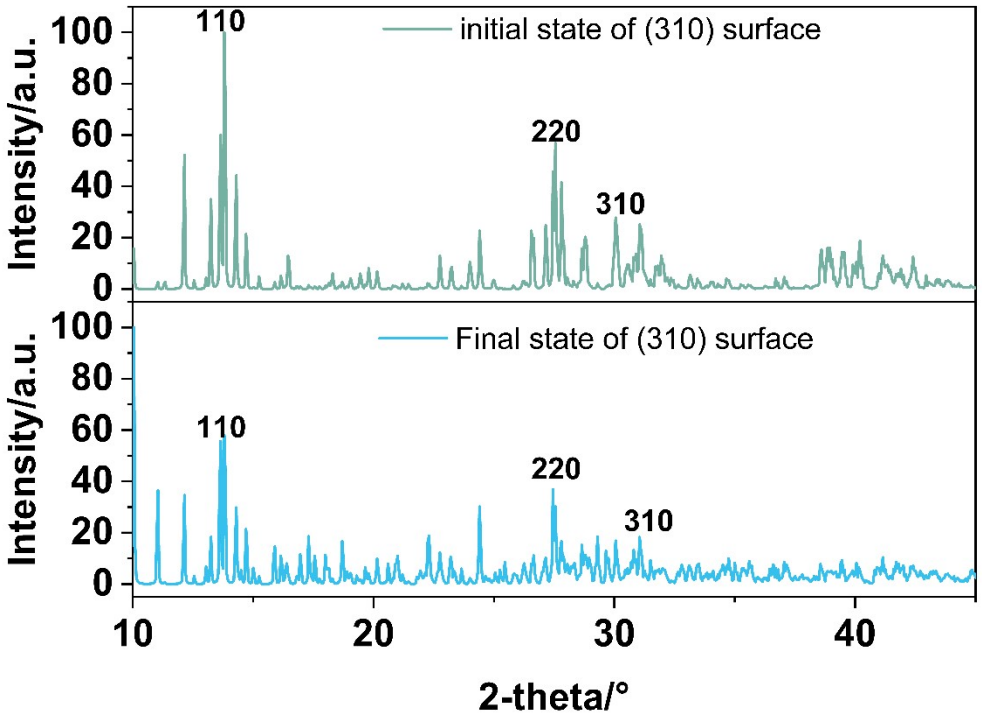

Figure S5 The XRD of (310) surface at 600 K